Absence of the diffusion pole in the Anderson insulator

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We discuss conditions for the existence of the diffusion pole and its consequences in disordered noninteracting electron systems. Using only nonperturbative and exact arguments we find against expectations that the diffusion pole can exist only in the diffusive (metallic) regime. We demonstrate that the diffusion pole in the Anderson localization phase would lead to nonexistence of the self-energy and hence to a physically inconsistent picture. The way how to consistently treat and understand the Anderson localization transition with vanishing of the diffusion pole is presented.

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The Anderson insulator is a specific disordered or amorphous solid with available quasiparticle states at the Fermi surface but with no diffusion or charge transport at long distances. Possibility of the absence of diffusion in impure metals and alloys was proposed by P. W. Anderson on a simple tight-binding model of disordered noninteracting electrons [1]. Since then, vanishing of diffusion, now called Anderson localization, has attracted much attention of both theorists and experimentalists [2]. In spite of a considerable portion of amassed experimental data, disclosed various specific and general aspects of the Anderson metal-insulator transition and a number of theoretical and computational approaches so far developed, we have not yet reached complete understanding of Anderson localization. Although the basic aspects of the critical behavior at the Anderson localization transition are known, the position of this disorder-driven metal-insulator transition within the standard classification scheme of phase transitions with control and order parameters remains yet unclear.

In this Letter we reexamine the description of Anderson localization with averaged functions. Configurational averaging is an important means to restore translational invariance in disordered systems and to provide reproducibility (sample independence) of the findings. Disordered systems after averaging behave as pure ones with effective correlations between the motion of individual quasiparticles. The translationally invariant description is hence the proper tool for comprehending the Anderson localization transition in the way we understand phase transitions in clean interacting systems.

The aim of the Letter is to set forth general constraints on the translationally invariant description of the Anderson localization transition resulting from exact relations, conservation laws and equations of motion for the averaged Green functions. We explicitly demonstrate that the weight of the diffusion pole cannot be fixed to unity as dictated by the Ward identity and that the diffusion pole must vanish in the localized phase. The diffusion pole in the localized phase would lead to nonexistence of the self-energy and to an unsolvable equation of motion for the two-particle vertex.

The fundamental building blocks of the translational invariant description of disordered electrons are averaged one and two-particle resolvents $G(\mathbf{k},z)$ and $G^{(2)}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q})$, respectively. Here $\mathbf{k},\mathbf{q}$ are fermionic and bosonic momenta and $z_\pm$ are complex energies. We use the electron-hole representation for the two-particle Green function with $\mathbf{k}$ and $\mathbf{k}'$ for incoming and outgoing electron momenta. The bosonic momentum $\mathbf{q}$ measures the difference between the incoming momenta of the electron and the hole.

Fundamental functions for the description of a linear response of an electron gas to an external electromagnetic perturbation are the density response and the electron-hole correlation function defined from the two-particle resolvent as

$$\chi(\mathbf{q},i\nu_m) = -\frac{1}{\beta N^2}\sum_{\mathbf{kk}'}\sum_{n=-\infty}^{\infty} G^{(2)}_{\mathbf{kk}'}(i\omega_n, i\omega_n + i\nu_m;\mathbf{q}), \tag{1a}$$

$$\Phi^{RA}_E(\mathbf{q},\omega) = \frac{1}{N^2}\sum_{\mathbf{kk}'} G^{(2)}_{\mathbf{kk}'}(E+\omega+i0^+, E-i0^+;\mathbf{q}) \ . \tag{1b}$$

For convenience, the density response χ was defined at the temperature axis, while the electron-hole correlation function Φ^{RA} for real frequencies. The superscript indices R,A relate to the limits of complex energies from which the first and second real energy variables were reached.

It is useful to go over from the full two-particle resolvent to a two-particle vertex Γ defined as

$$\begin{aligned} G^{(2)}_{\mathbf{kk}'}(z_+,z_-;\mathbf{q}) &= G(\mathbf{k}+\mathbf{q},z_+)G(\mathbf{k},z_-)\,[1 \\ &\quad + \Gamma_{\mathbf{kk}'}(z_+,z_-;\mathbf{q})G(\mathbf{k}'+\mathbf{q},z_+)G(\mathbf{k}',z_-)] \ . \end{aligned} \tag{2}$$

The two-particle vertex obeys a Bethe-Salpeter equation of motion. Since we use the electron-hole representation, the most natural way to construct the Bethe-Salpeter equation is to use ladders in the electron-hole scattering

channel. We then can write

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Lambda^{eh}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \frac{1}{N}\sum_{\mathbf{k}''}\Lambda^{eh}_{\mathbf{k}\mathbf{k}''}(\mathbf{q})G_+(\mathbf{k}''+\mathbf{q})G_-(\mathbf{k}'')\Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) \quad (3)$$

where we introduced the electron-hole irreducible vertex Λ^{eh}. We suppressed the energy variables in Eq. (3), since they are not dynamical quantities and act only as external parameters. They are easily deducible from the one-electron propagators $G_\pm(\mathbf{k}) \equiv G(\mathbf{k}, z_\pm)$.

We have up to now used only definitions or representations of the two-particle functions. The first important equation demanding a proof is the Vollhardt-Wölfle identity expressing conservation of the norm of the wave function of a free electron scattered on a static impurity potential

$$\Sigma^R(\mathbf{k}, E+\omega) - \Sigma^A(\mathbf{k}, E) = \frac{1}{N}\sum_{\mathbf{k}'}\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) \times \left[G^R(\mathbf{k}', E+\omega) - G^A(\mathbf{k}', E)\right] \ . \quad (4)$$

Here we denoted Σ^R, Σ^A the retarded and advanced self-energy and $\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) \equiv \Lambda^{eh}_{\mathbf{k}\mathbf{k}'}(E+\omega+i0^+, E-i0^+; \mathbf{0})$. Equation (4) was proved diagrammatically in Ref. [3]. A nonperturbative proof exists trough equivalence of Eq. (4) with the Velický identity [4, 5]. We hence can consider Eq. (4) as a nonperturbative property of solutions of the Anderson model of disordered electrons [6].

The first fundamental consequence of Eq. (4) is the existence of the diffusion pole in the electron-hole correlation function Φ^{RA}. Introducing a quantum diffusion function $D(\mathbf{q},\omega)$ we can represent the density response in the hydrodynamic limit $q \to 0$ as [7]

$$\chi(\mathbf{q},\omega) \doteq \frac{\chi_0 D(\omega) q^2}{-i\omega + D(\omega)q^2} + O(q^2) \quad (5)$$

where $\chi_0 = \lim_{q\to 0}\lim_{\omega\to 0}\chi(\mathbf{q},\omega)$ and $D(\omega) = D(\mathbf{0},\omega)$. The dynamical diffusion coefficient $D(\omega)$ reduces in the static limit to the diffusion constant related at zero temperature to the static optical conductivity by the Einstein formula $D = D(0) = \sigma/e^2 n_F$, where n_F is the density of states at the Fermi energy [7].

Using Eqs. (1) we can now expand the density response in the hydrodynamic ($q \to 0$) and quasistatic ($\omega \to 0$) limits maintaining $D(\omega)q^2 \sim \omega$. We find that its leading term at zero temperature is governed by the electron-hole correlation function

$$\chi(\mathbf{q},\omega) = \chi(\mathbf{q},0) + \frac{i\omega}{2\pi}\left(\Phi^{RA}_E(\mathbf{q},\omega) + O(q^0)\right) + O(\omega) \ . \quad (6)$$

Inserting the asymptotic expansion Eq. (6) in Eq. (5) we derive an explicit representation of the diffusion pole as the leading low-energy term in the electron-hole correlation function

$$\Phi^{RA}_E(\mathbf{q},\omega) \doteq \frac{2\pi n_F}{-i\omega + D(\omega)q^2} + O(q^0,\omega^0) \ . \quad (7)$$

Although the denominator in the density response in Eq. (5) is identical with that from the electron-hole correlation function in Eq. (7), it is only the latter function that is singular in the low-energy limit. This singularity, the diffusion pole, is a consequence of the particle-number conservation expressed mathematically in the Ward identity (4). The only parameter depending on the character of the underlying solution in Eq. (7) is the dynamical diffusion coefficient $D(\omega)$. This simplified low-energy asymptotics of the electron-hole correlation function is the basis for the existing scaling and field-theoretic approaches to the problem of Anderson localization [8].

According to the above reasoning the diffusion pole must exist also in the state with localized electrons, where the dynamical diffusion coefficient is expected to vanish in the static limit as [3]

$$D(\omega) \sim -i\omega\xi^2 \quad (8)$$

where ξ is the localization length. We, however, show that such a picture is not sustainable, since the diffusion pole in the localized phase would hinder the existence of a finite self-energy almost everywhere within the energy band.

To manifest this we first show that in systems invariant with respect to time reversal the diffusion pole enters the electron-hole irreducible vertex Λ^{eh} as the so-called Cooper pole. It displays the same low-energy asymptotics as the electron-hole correlation function Φ^{RA}.

Time inversion in noninteracting systems with elastic scatterings only is expressed as inversion of the particle propagation $\mathbf{k} \to -\mathbf{k}$, i. e., the electron and hole interchange their roles. The time-reversal invariance then means that $G(\mathbf{k},z) = G(-\mathbf{k},z)$. For the two-particle resolvent we then obtain either $G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = G^{(2)}_{-\mathbf{k}'-\mathbf{k}}(z_+,z_-;\mathbf{q}+\mathbf{k}+\mathbf{k}')$ or equivalently $G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;\mathbf{q}) = G^{(2)}_{\mathbf{k}\mathbf{k}'}(z_+,z_-;-\mathbf{q}-\mathbf{k}-\mathbf{k}')$ leading to $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Gamma_{-\mathbf{k}'-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}')$. However, the electron-hole irreducible vertex Λ^{eh} is not invariant in the same way the full two-particle vertex Γ is. We actually have $\Lambda^{eh}_{-\mathbf{k}'-\mathbf{k}}(\mathbf{q}+\mathbf{k}+\mathbf{k}') = \Lambda^{ee}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$, where Λ^{ee} is the electron-electron irreducible vertex being generally different from the electron-hole one. The Bethe-Salpeter equation (3) after time reversal is hence transformed to another Bethe-Salpeter equation with the electron-electron irreducible vertex and modified momentum convolutions. The existence of several Bethe-Salpeter equations for the same full two-particle vertex Γ is a well known ambiguity in the definition of the two-particle irreducibility [5].

The low-energy singularity in the electron-hole correlation function is a consequence of the existence of a

singularity in the full two-particle vertex Γ^{RA}, since the former function is the latter one multiplied with one-electron propagators and summed over fermionic momenta, cf. Eqs. (1b) and (2). It means that $\Gamma^{RA}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ diverges with $\omega, \mathbf{q}^2 \to 0$ for almost all fermionic momenta $\mathbf{k}, \mathbf{k}'$ so that its singularity survives in Φ^{RA} as the diffusion pole, Eq. (7). However, due to the electron-hole symmetry, the full two-particle vertex must show the same singularity also in the limit $\omega, (\mathbf{k} + \mathbf{k}' + \mathbf{q})^2 \to 0$.

Further on, the (leading) singularities in the full vertex Γ are already contained in the irreducible vertices Λ^{eh} and Λ^{ee}. This conclusion follows from the so-called parquet equation. It is an expression of topological nonequivalence of different two-particle irreducibilities. That is, the reducible function of one type (convolution of two or more irreducible vertices of the same type) is irreducible in the other irreducibility channels. In case of two irreducibility channels (two types of Bethe-Salpeter equations) we can write the parquet equation as

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Lambda^{ee}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) + \Lambda^{eh}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \ . \tag{9}$$

where $\mathcal{I} = \Lambda^{eh} \cap \Lambda^{ee}$ is a vertex irreducible in both irreducibility channels (completely irreducible vertex) [5].

We deduce the form of the pole in the electron-hole irreducible vertex Λ^{eh} from the asymptotic limit to high spatial dimensions [9]. There we obtain that the completely irreducible vertex $\mathcal{I}$ is local and regular. The singularity of the full vertex Γ^{RA} in the limit $\omega, \mathbf{q}^2 \to 0$ is contained in the electron-electron irreducible vertex, Λ^{ee}, while the singularity for $\omega, (\mathbf{k} + \mathbf{k}' + \mathbf{q})^2 \to 0$ appears only in Λ^{eh}. The low-energy singularities of the irreducible vertices are fixed in momentum space by the asymptotics $d \to \infty$ if this limit is analytic for the two-particle functions. Since the neglected contributions to the two-particle vertex are less singular than the leading divergent $d \to \infty$ terms containing the diffusion and Cooper poles, we can assume analyticity of the high-dimensional limit, even if we cannot prove it rigorously. Using the high dimensional separation of singularities of the full vertex into the irreducible ones we obtain from Eq. (7) at zero temperature for $q = 0$

$$\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) = \lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) + \frac{2\pi n_F \lambda}{-i\omega + D(\omega)(\mathbf{k} + \mathbf{k}')^2} \tag{10}$$

where λ is a measure of the disorder strength. The function $\lambda^{RA}_{\mathbf{k}\mathbf{k}'}$ is nonsingular or at least less singular than the Cooper pole singled out from the electron-hole irreducible vertex, second term on the r.h.s. of Eq. (10). Notice that the asymptotic form of the Copper pole in Eq. (10) is exact only if the the Ward identity (4) is obeyed. The Cooper pole in Eq. (10) is the generally anticipated singularity of the electron-hole irreducible vertex [3].

To test consistence of such singular behavior of the electron-hole irreducible vertex we define a difference of two retarded self-energies

$$\Delta W_E(\omega) = \frac{1}{N} \sum_{\mathbf{k}} [\Sigma^R(\mathbf{k}, E-\omega) - \Sigma^R(\mathbf{k}, E+\omega)] \ . \tag{11a}$$

We will be interested in its low-frequency behavior, i. e., the asymptotic limit $\lim_{\omega\to 0} \Delta W_E(\omega)$. If the self-energy $\Sigma^R(E)$ is an analytic function of the energy variable E, which normally is the case within the energy bands, then $\Delta W_E(\omega)$ must be analytic at $\omega = 0$ for almost all energies E for which $\Im \Sigma^R(E) > 0$. If the self-energy is a continuous function of the energy argument, then $\Delta W_E(0) = 0$. Finiteness of the derivative of the self-energy demands $\lim_{\omega\to 0} |\Delta W_E(\omega)/\omega| < \infty$, etc.

We apply the Ward identity (4) to represent the r.h.s. of Eq. (11a) via the electron-hole irreducible vertex. We obtain

$$\begin{aligned}
\Delta W_E(\omega) = \frac{-1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} & \{2i \\
& \times \left[\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) - \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E-\omega, E)\right] \Im G^R(\mathbf{k}', E) \\
& + \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) \left[G^R_{\mathbf{k}'}(E+\omega) - G^R_{\mathbf{k}'}(E)\right] \\
& - \Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E-\omega, E) \left[G^R_{\mathbf{k}'}(E-\omega) - G^R_{\mathbf{k}'}(E)\right]\} \ .
\end{aligned} \tag{11b}$$

We use representation (10) for the electron-hole irreducible vertex to derive the low-frequency asymptotics $\lim_{\omega\to 0} \Delta W_E(\omega)$. Actually we are interested only in the most singular part being generated by the Cooper pole. It is a straightforward task to perform momentum integration on a d-dimensional hypercubic lattice leading to [10]

$$\Delta W^{sing}_E(\omega) \approx K_d \lambda n_F^2 \times \begin{cases} \frac{1}{\omega} \left|\frac{\omega}{D(\omega) k_F^2}\right|^{d/2} & \text{for } d \neq 4l, \\ \frac{1}{\omega} \left|\frac{\omega}{D(\omega) k_F^2}\right|^{d/2} \ln\left|\frac{D(\omega) k_F^2}{\omega}\right| & \text{for } d = 4l. \end{cases} \tag{12}$$

In the diffusive phase, $D(\omega) = D > 0$, that realizes only for $d > 2$, we find nonexistence of derivatives of the self-energy independently of the energy position within the band. Realization of a self-energy with nonexisting (diverging) $[(d-2)/2]$th derivative everywhere is apparently unphysical for $d < \infty$.

The situation worsens if we evaluate $\lim_{\omega\to 0} \Delta W_E(\omega)$ for the localized solution with the low-frequency dynamical diffusion function from Eq. (8). We then obtain independently of the spatial dimension $\Delta W^{sing}_E(\omega) \sim C_d/\omega$. This is a catastrophe indicating nonexistence of the retarded self-energy as a well defined mathematical function. This may not happen. Hence, our picture based on the Ward identity (4) resulting in the Cooper pole in the electron-hole vertex, Eq. (10), is inconsistent. The real solution of the Anderson model must behave differently from the above derived singular behavior.

The correct low-energy behavior of the electron-hole vertex can be assessed from the exact asymptotic solution in high spatial dimensions. The limit to high spatial dimensions leads to simplifications in momentum convolutions so that one can solve the parquet equations for the irreducible vertices Λ^{eh} and Λ^{ee} asymptotically exactly [9]. In this asymptotic solution the Ward identity (4) is not obeyed for nonzero real energy differences $\omega \neq 0$. A deviation from the Ward identity leads to a modified diffusion (Cooper) pole. In the localized phase we then obtain for $\omega, (\mathbf{k}+\mathbf{k}')^2 \to 0$ the electron-hole irreducible vertex in the asymptotic form

$$\Lambda^{RA}_{\mathbf{k}\mathbf{k}'}(E+\omega, E) \approx \frac{i}{A(\omega)\omega} \, \frac{2\pi n_F \lambda}{1+\xi^2(\mathbf{k}+\mathbf{k}')^2} \tag{13}$$

where $\xi^2 = iD(\omega)/A(\omega)\omega$ is the square of the localization length. The limit $\lim_{\omega\to 0} A(\omega)\omega$ becomes finite inside the localized phase as well as the localization length ξ. We can see from Eq. (13) that the electron-hole irreducible vertex does not display a low-energy singularity. It means that there is also no diffusion pole in the electron-hole correlation function in the localized phase. This is a necessary condition for the existence of the self-energy as a well behaved function along the real axis of the energy variable (Fermi energy).

The fraction $|1/A(\omega)| \leq 1$ generally determines the weight of the diffusion pole. The static value $A(0)$ is finite in the diffusive phase, increases with the disorder strength and diverges at the Anderson localization transition. The renormalized density of states $n_F/A(0)$ represents the number of diffusive states, that is, extended states being able to carry electron charge to long distances. These are the only states contributing to charge transport, whereas n_F is the density of all available states at the Fermi energy E_F.

Nonconservation of the averaged particle density incurred by a violation of the Ward identity (4) in the high-dimensional solution for the vertex function is a consequence of the configurational averaging [11]. Validity of Eq. (4) is conditioned by completeness of Bloch waves for all relevant configurations of the random potential. During the configurational averaging we lose the spatially restricted localized states in the thermodynamic limit. To form a representation Hilbert space we have to fix boundary conditions for the eigenstates of the random Hamiltonian. The extended states vanish at the volume boundary as $V^{-1/2}$, while the localized states vanish exponentially $\exp\{-V/v_0\}$. The two types of states are orthogonal in the thermodynamic limit. Restoring translational invariance restricts our description only to states extended over the whole volume. The only localized states surviving configurational averaging are the periodically repeated ones. If there is a macroscopic portion of configurations with spatially bounded states breaking translational invariance near the Fermi energy, the number of available translational invariant states is less than the total number of states. Hence, the probability to find the electron in an extended state is less than one.

To conclude, we showed that the diffusion pole in the electron-hole correlation function cannot survive beyond the mobility edge where all states become localized. We used only exact and nonperturbative arguments and found incompatibility of the Ward identity (4), implying a singular low-energy asymptotics of the electron-hole correlation function, Eq. (7), with the existence of the retarded self-energy as a well defined function of the energy variable. We demonstrated that a necessary condition for the existence of a regular (finite) self-energy in the localized phase is regularity of the electron-hole irreducible vertex in the low-energy limit. Supported by the asymptotic solution of the Anderson model in high spatial dimensions we concluded that the weight of the diffusion pole in the metallic regime is $1/A(0) \leq 1$. This weight decreases with increasing disorder strength and vanishes at the localization transition. The most striking consequence of our finding is that it is not the diffusion constant $D(0)$ but the weight of the diffusion pole $1/A(0) \leq 1$ that is the relevant control parameter for the Anderson localization transition.

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